

Cometary X-ray emission: theoretical cross sections following charge exchange by multiply charged ions of astrophysical interest¹

S. Otranto, R.E. Olson, and P. Beiersdorfer

Abstract: The classical trajectory Monte Carlo (CTMC) method is used to calculate emission cross sections following charge exchange collisions involving highly charged ions of astrophysical interest and typical cometary targets. Comparison is made to experimental data obtained on the EBIT machine at Lawrence Livermore National Laboratory (LLNL) for O^{8+} projectiles impinging on different targets at a collision energy of 10 eV/amu. The theoretical cross sections are used together with ion abundances measured by the Advanced Composition Explorer as well as those obtained by a fitting procedure using laboratory emission cross sections to reproduce the X-ray spectrum of comet C/LINEAR S4 measured on 14 July 2001.

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Résumé : Nous utilisons la méthode CTMC pour calculer les sections efficaces d'émission suivant des collisions par échange de charge impliquant des ions hautement chargés intéressants en astrophysique, sur des cibles typiques de matériaux trouvés dans une comète. Nous comparons avec les mesures expérimentales obtenues par l'appareil EBIT au Lawrence Livermore National Laboratory (LLNL) pour des projectiles de O^{8+} sur différentes cibles à une énergie de collision de 10 eV/amu. Nous utilisons les sections efficaces calculées avec les données d'abondance ionique du Advanced Composition Explorer ainsi qu'avec celles obtenues par ajustement numérique utilisant les données prises en laboratoire afin de reproduire le spectre-X de la comète C/LINEAR S4 mesuré le 14 juillet 2001.

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1. Introduction

X-ray emission from comets has recently been observed and has had a great impact not only because the intensity of the emission was unexpected but because of the richness on the underlying atomic physics [1, 2]. Even though the spectral resolution in the initial observations was not good enough to clarify the origin of such emission, nowadays, it is widely accepted that the X-ray emission from comets originates in charge exchange processes between the solar wind ions and the cometary coma gases [3].

Quantum mechanical methods like the continuum distorted wave (CDW) [4], or CDW-eikonal initial state (EIS) [5] have been successfully used to study single electron capture from light targets for many years in the high collision energy limit.

On the other hand, the low impact energy region still represents a challenge for theoreticians. Quantum mechanical methods such as the atomic and molecular orbital methods provide accurate values for light-target systems such as atomic H and He for low impact energies at the expense of large basis sets [6]. Simpler methods like the multichannel Landau-Zener (LZ) [7] and CTMC [8], on the other hand, provide reasonable results for complex systems such as molecular targets or highly charged projectiles.

Within the CTMC method semiclassical methods have been developed to predict the n , l , and m electron capture excited levels. By following the dipole-allowed photon transitions as they de-excite to the ground state, the emission cross sections are obtained. For almost 20 years, the CTMC line emission cross sections for the H target have been used for diagnostics on tokamak fusion plasmas to determine the concentrations of highly charged impurity ions in the energy range of 1 to 40 keV/amu [9, 10]. More recently, CTMC emission lines have been presented for collisions involving partially and fully stripped ions with Li, providing an accurate description of the measured data [11].

In the present paper, we present emission lines for typical solar-wind highly charged ions colliding with cometary targets using a one-active electron representation of the problem. We consider the cometary gases as hydrogenic atoms with their corresponding ionization potentials (IP). Our theoretical results are first compared to high-resolution data obtained with the EBIT machine at LLNL at low collision energies (10 eV/amu) [12]. Then, they are compared with data measured for similar

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reactions but for impact energies that are in accord with the astrophysical observations ($\sim 1\text{--}3$ keV/amu) [13, 14].

Furthermore, we use the calculated emission cross sections together with the ion abundances measured by the Advanced Composition Explorer (ACE) to predict cometary spectra.

2. Experimental details

Our measurements were carried out at the Lawrence Livermore EBIT-I electron ion trap, making use of the magnetic trapping mode of operation [15, 16]. The electron beam was turned off after production of highly charged ions and EBIT was operated like a Penning trap. Ions were confined radially by a 3 T magnetic field generated by superconducting Helmholtz coils and longitudinally by the potential applied to the outer electrodes of the cylindrical trap. From the preceding conditions, the temperature of the ions was estimated to be about 10 ± 4 eV/amu.

Since ions were created in situ in EBIT, transfer loss was avoided and as many as 10^7 ions were produced. Electron capture was induced by ballistic injection of gases either in a continuous mode [15] or in a pulsed mode [17]. X-ray spectra were recorded using a high-resolution microcalorimeter.

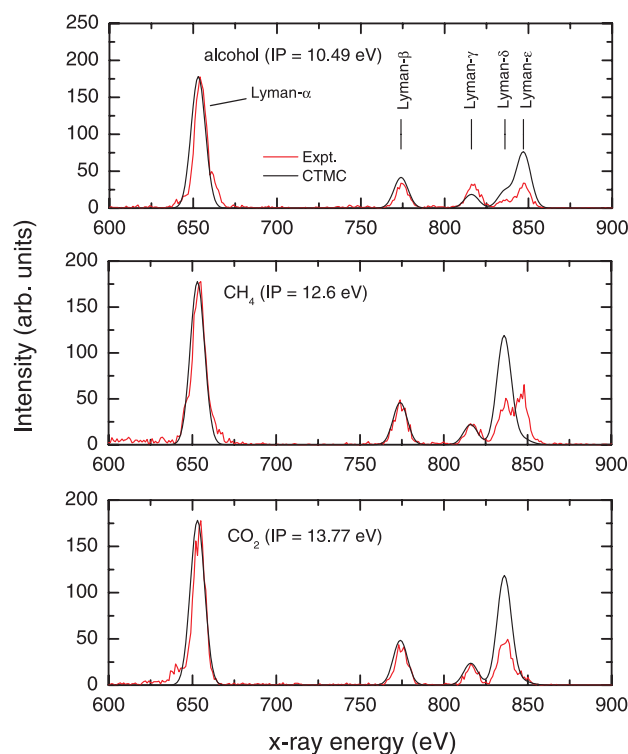
The spare X-ray microcalorimeter spectrometer (XRS) from the ASTRO-E satellite mission was used. The XRS consists of a 6×6 pixel array with 32 active channels, forming a combined active area of 13 mm^2 that is operated at 59 mK [18]. Its energy resolution (better than 10 eV) is an order of magnitude better than traditional Ge or SiLi detectors, and allowed us to distinguish discrete lines associated with $np \rightarrow 1s$ Lyman X-ray transitions following electron capture [13, 19].

3. Results

The LZ and CTMC methods predicted early on that the total cross section for the single electron capture from H scaled linearly with the impinging charge and was energy independent for highly charged projectiles ($\sigma \sim q \times 10^{-15} \text{ cm}^2$) for collision energies below about 10 keV/amu. Further CTMC calculations showed in 1981 that the most probable principal quantum number for capture was $n_p = n_i q^{3/4}$, where n_i is the initial level of a H target and q the projectile charge state. Within the hydrogenic approximation used throughout this article, the latter equation can be generalized as $n_p = (13.6 \text{ eV/IP})^{1/2} q^{3/4}$.

One of the advantages of the CTMC method is that it inherently provides the population of the l -levels for each n -level, which is vital for obtaining the corresponding emission cross sections. Other treatments [20, 21] have been either based on the assumption of the high-energy statistical limit in which all the emission can be assumed to be due to the $n = 2 \rightarrow 1$ transition, or equally probable emissions from $n = 2, \dots, n_p$ to the ground state. While the former assumption clearly underestimates the higher Lyman lines, the latter tends to overestimate the higher Lyman lines and does not show any kind of energy-dependence for the Lyman lines. It was shown by Beiersdorfer et al. in 2001 that these two models fail to predict the shape of the emission cross sections following Ne^{10+} and Ne^{9+} collisions on Ne, and that discrepancies become clearly

Fig. 1. Data obtained with the EBIT machine at LLNL and a 10 eV resolution XRMS for 10 eV/amu O^{8+} collisions on alcohol, CH_4 and CO_2 . The CTMC emission lines presented for the same systems have been normalized to the Ly- α peak.



visible even considering data obtained with EBIT-II by means of a Ge detector (energy resolution FWHM = 235 eV) [19]. On the other hand, the predictions of the CTMC method are in good agreement with the data for both systems [12].

In Fig. 1, we show the emission cross sections measured by Beiersdorfer et al. with the EBIT machine and a 10 eV resolution microcalorimeter spectrometer (XRMS) like the one that is on the Suzaku X-ray Observatory and that, unfortunately, failed after only a few weeks of operation. The relative experimental data obtained for 0.01 keV/amu collisions of O^{8+} with alcohol, CH_4 and CO_2 are shown. It can be seen that the Ly- α , Ly- β , and Ly- γ peaks are similar for all the targets but the Ly- δ and Ly- ϵ representing the $5p \rightarrow 1s$ and $6p \rightarrow 1s$ transitions seem to be target dependent. Similar trends are followed by the CTMC (degraded to 10 eV resolution) even though for CH_4 the $6p \rightarrow 1s$ transition seems to be absent and the experiment shows that the emission is as strong as that coming from the $5p \rightarrow 1s$ transition. The present results are in agreement with the above shown equation for the most probable n_p , which predicts that electrons captured from targets with lower binding energies will populate higher n values.

In Fig. 2, we use the calculated emission cross sections to reproduce the spectrum of comet C/Linear 1999 S4. The ACIS-S effective area has been considered. The abundances for the $\text{C}^{5+,6+}$ and $\text{O}^{7+,8+}$ projectiles have been obtained from ACE measurements that are tabulated in 2 h averages [22] while for $\text{N}^{6+,7+}$ we have used tabulated values corresponding to the slow solar wind [23]. Due to the time delay in the solar

Fig. 2. Spectrum of C/LINEAR 1999 S4 corresponding to 14 July 2001. Theories: continuous line, CTMC-ACE; broken line, CTMC-EBIT fit; and dot-dash-line, CTMC-EBIT using the lowest estimated limit for the C^{5+} abundance.

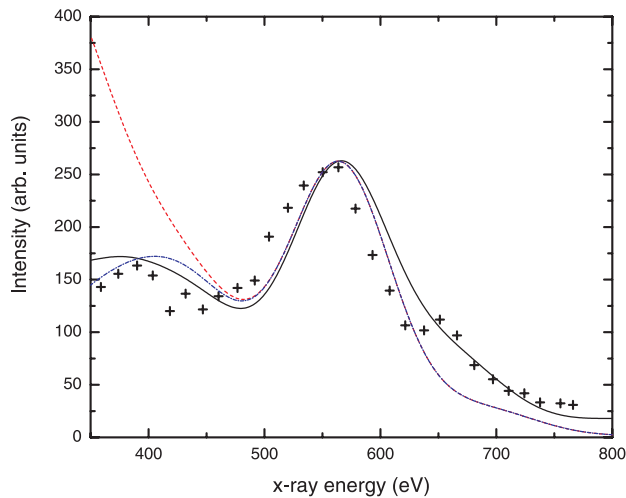


Table 1. Comparison of ion abundances obtained by Beiersdorfer et al. [24] by fitting the S4 spectrum with 10 eV/amu EBIT cross sections with those measured by the ACE and corresponding to the estimated full delay (+0.7 days) [2]. For $N^{6+.7+}$ the slow solar wind abundances tabulated by Schwadron and Cravens [23] have been considered.

Ion/[X^{Q+}/O^{7+}]	Ref. 24	ACE
C^{5+}	11 ± 9	0.869
C^{6+}	0.9 ± 0.3	1.26
N^{6+}	0.5 ± 0.3	0.25 (Schwadron and Cravens)
N^{7+}	0.06 ± 0.02	0.026 (Schwadron and Cravens)
O^{7+}	1 ± 0.04	1
O^{8+}	0.13 ± 0.03	0.174

wind events measured by the ACE and the comet, the spectrum obtained according to the estimated full delay (+0.7 days) [2] is shown. For comparison, we present the CTMC results when the abundances obtained by Beiersdorfer et al. [24] (by fitting the S4 spectrum by means of the 10 eV/amu EBIT laboratory cross sections) are considered (see Table 1). Since in ref. 24, ratios of abundances to the O^{7+} were provided, we normalized the O^{7+} abundance to the ACE value. Overall, Table 1 confirms that the EBIT-based measurements provide a very reasonable prediction of solar wind abundances, as evidenced by the ion compositions reported later in the ACE satellite data.

4. Conclusions

In this work we have benchmarked CTMC emission lines with high-resolution experimental data obtained on the EBIT machine at LLNL. The calculated emission lines correctly predict that for low impact energies the intensity of the higher Lyman lines depend on the ionization potential of the target.

The high-resolution results obtained on the EBIT machine

during the last decade have represented a major step to our understanding of the emission cross sections and helped to rule out emission models that were based on imprecise assumptions on how the l -levels were populated during the charge exchange.

It is worth mentioning then that the present theoretical model inherently accounts for the captured electron population of the different l -levels at different impact energies and has provided the closest theoretical agreement to date to the EBIT data.

Finally, we have shown that the calculated cross sections together with ACE measured abundances corresponding to the estimated full delay lead to a spectrum in good agreement with that measured on 14 July 2000 for the C/LINEAR comet.

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